Harmonic Oscillator Problem

1. Classical vs. Quantum Harmonic Oscillators (HO)
2. Brute – Force Treatment of Quantum HO
3. Treatment of Quantum HO with Operators
4. Motion in a Magnetic Field

Classical Versus Quantum Harmonic Oscillators Examples

Simple Harmonic Motion

- Simple harmonic motion (SHM) refers to a certain kind of oscillatory, or wave-like motion that describes the behavior of many physical phenomena:
  - a pendulum
  - a bob attached to a spring
  - low amplitude waves in air (sound), water, the ground
  - the electromagnetic field of laser light
  - vibration of a plucked guitar string
  - the electric current of most AC power supplies
  - …

Simple harmonic motion

- SHM is pure "sinusoidal" motion, i.e. the relevant property described by SHM (displacement, pressure, current, etc.) is a sine wave:

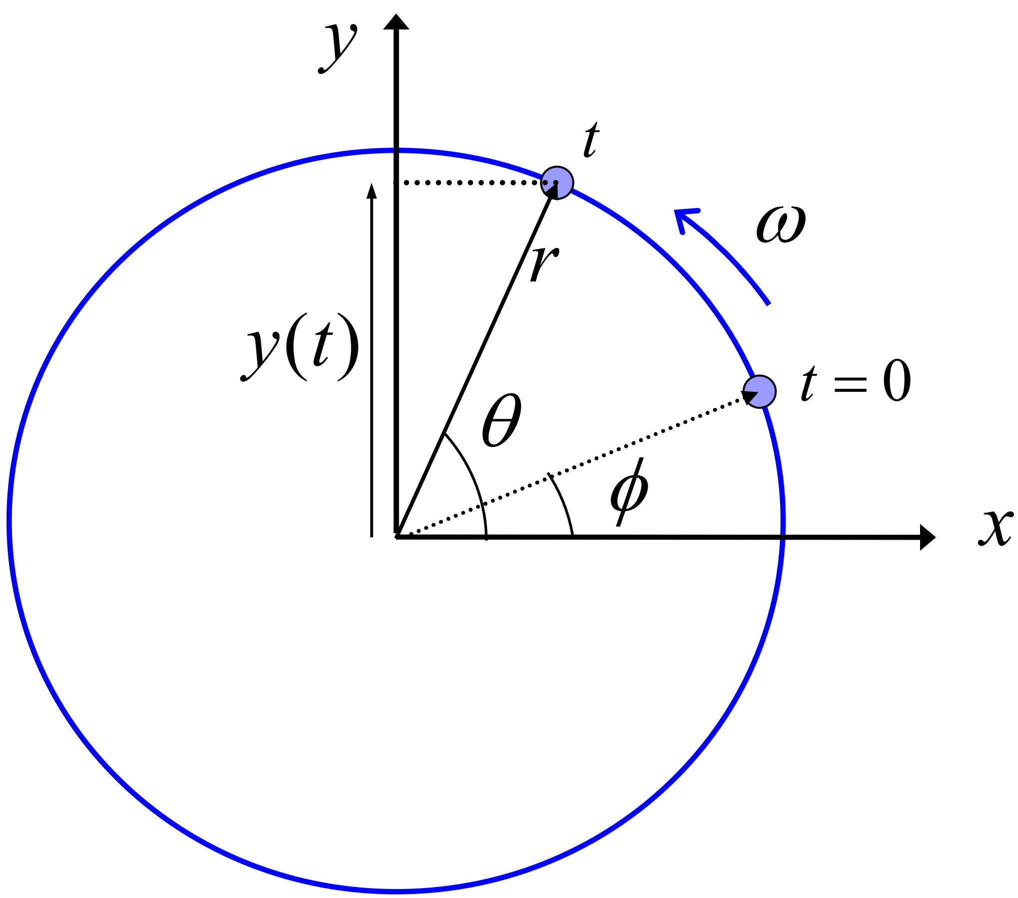
$$p(t) = A\sin(\omega t + \phi)$$

- ω is the *angular frequency* of the wave (in radians per second), A is its *amplitude*, and ϕ is the *initial phase* of the wave (in radians).

- the units of p are whatever those of A are

Example: the projection of uniform circular motion

- consider an object undergoing uniform circular motion:



- lets look at the *projection* of this motion on the y axis; in other words, we want $y(t)$. From the diagram:

$$y = r\sin(\theta)$$

- the angular displacement at time t is

$$\theta = \omega t + \phi$$

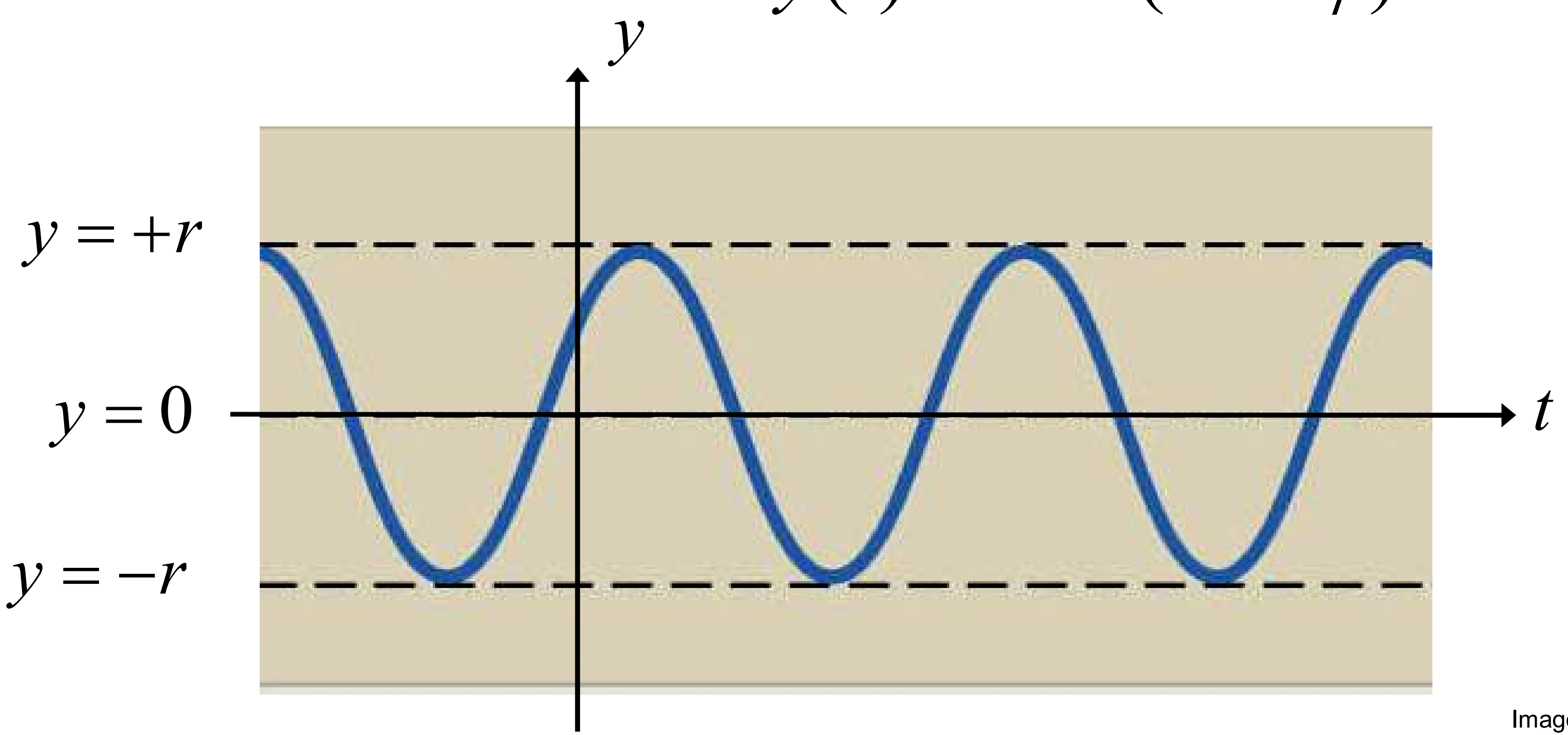
- and so,

$$y(t) = r\sin(\omega t + \phi)$$

simple harmonic motion!

Example: the projection of uniform circular motion

$$y(t) = r\sin(\omega t + \phi)$$



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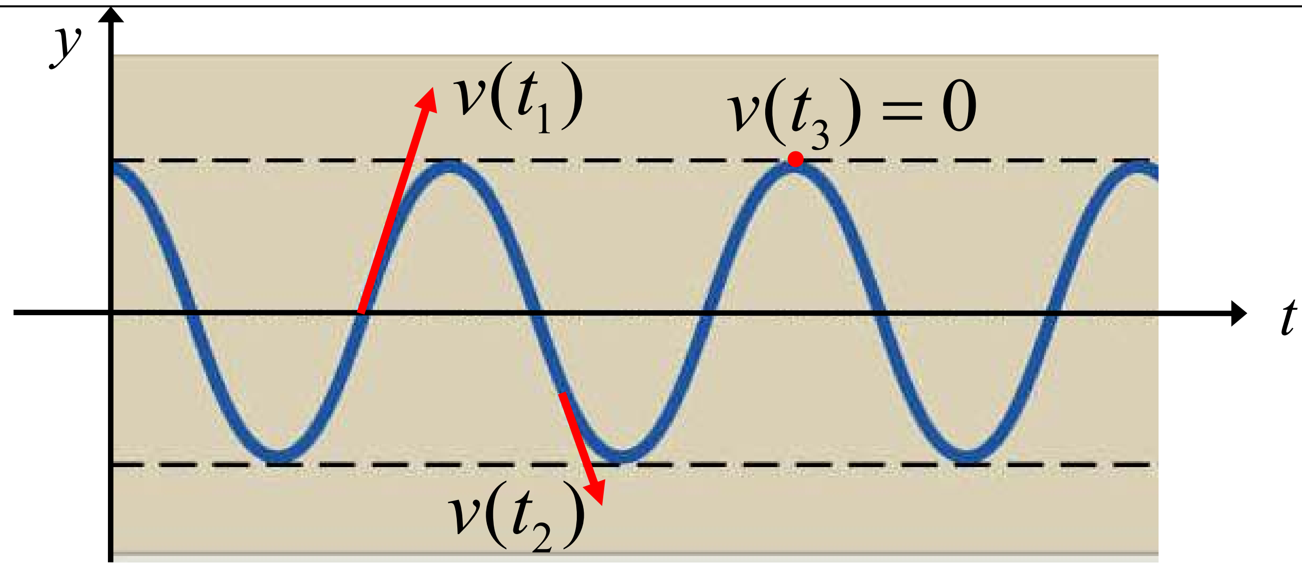
Velocity and acceleration in SHM

- The position of an object undergoing SHM changes with time, thus it has a velocity
- Recall that the velocity of an object is the *slope* of its graph of position vs. time. Thus, we can see that velocity in SHM also changes with time, and so object is accelerating:



Velocity and acceleration in SHM

- We can use the uniform circular motion model to deduce what the velocity and acceleration with time are (or using calculus, which is actually easier in this case!). Here are the results:

$$y(t) = r\sin(\omega t + \phi)$$

$$v(t) = r\omega\cos(\omega t + \phi)$$

$$a(t) = -r\omega^2\sin(\omega t + \phi)$$

Velocity and acceleration in SHM

- Sometimes it's easier to work with $\cos$ for position rather than $\sin$. Since we have an arbitrary phase in SHM (we can choose whatever we want for t=0), we can always define a new phase:

$$\phi = \psi + \pi / 2$$

- Then using the following trig identities

$$\cos(\theta + \pi / 2) = -\sin(\theta), \quad \sin(\theta + \pi / 2) = \cos(\theta)$$

we find: *(be careful with the signs!)*

$$\begin{aligned} y(t) &= r\sin(\omega t + \phi) \\ v(t) &= r\omega\cos(\omega t + \phi) \\ a(t) &= -r\omega^2 \sin(\omega t + \phi) \end{aligned} \quad \Leftrightarrow \quad \begin{aligned} y(t) &= r\cos(\omega t + \psi) \\ v(t) &= -r\omega\sin(\omega t + \psi) \\ a(t) &= -r\omega^2 \cos(\omega t + \psi) \end{aligned}$$

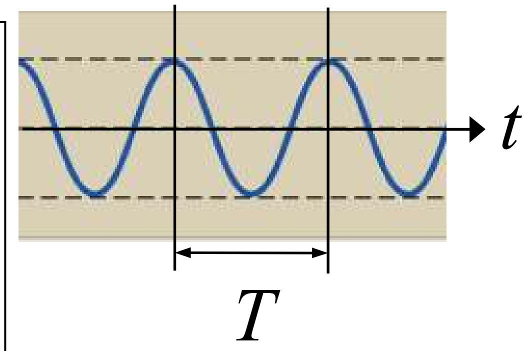
The period and frequency of a wave

- the period T of a wave is the amount of time it takes to go through 1 cycle
- the frequency f is the number of cycles per second
  - the unit of a cycle-per-second is commonly referred to as a hertz (Hz), after Heinrich Hertz (1847-1894), who discovered radio waves.
- frequency and period are related as follows:

$$f = \frac{1}{T}$$

- Since a cycle is 2π radians, the relationship between frequency and angular frequency is:

$$\omega = 2\pi f$$

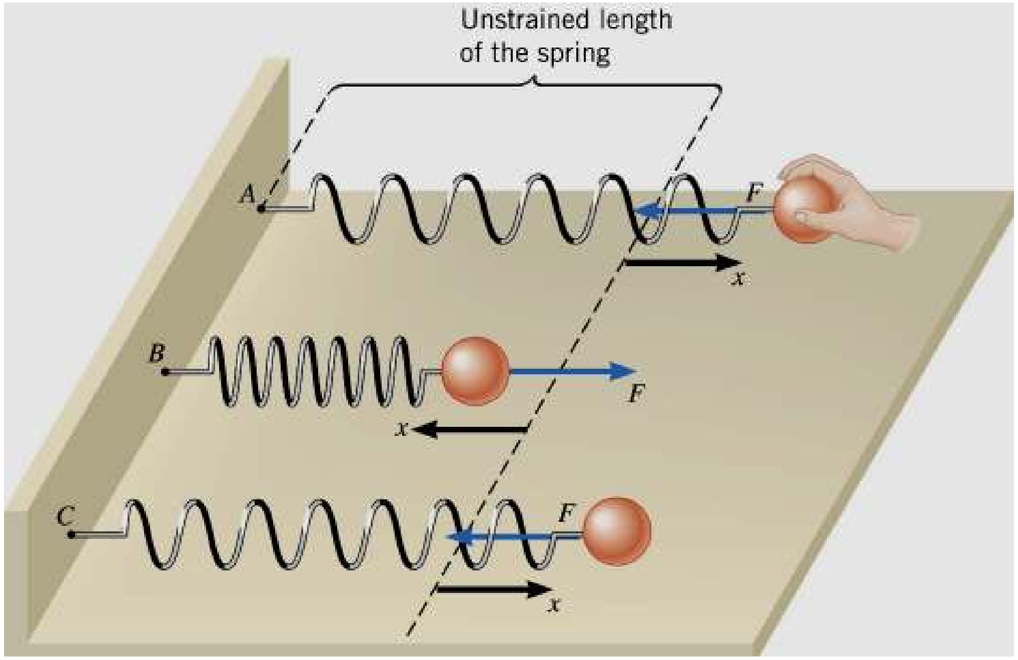


HEINRICH RUDOLF HERTZ
1847 - 1894

Springs

- A spring is a familiar device of everyday life. The basic property of a spring is that it resists any deviation from its unstrained configuration, and the further the deviation, the greater the force of resistance.

- The force a spring exerts to try to return it to its unstrained state is called the restoring force.



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The Ideal Spring

- The ideal spring is a simple mathematical model of the behavior of a spring:

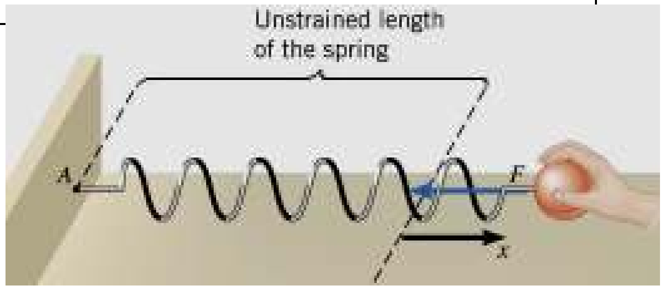
$$F = -kx$$

F is the restoring force exerted by a spring whose end-point is a distance x away from its equilibrium configuration. κ is called the spring constant, and has units of N/m. k describes how "stiff" the spring is.

- For an ideal spring, we also consider it to be *massless*

- The above equation is known as Hooke's Law (after Robert Hooke (1635-1703), an inventor, philosopher, architect, ...)

- Hooke's law is a good characterization of a spring for small displacements



Springs and simple harmonic motion

- Attach an object of mass m to the end of a spring, pull it out to a distance A, and let it go from rest. The object will then undergo simple harmonic motion:

$$x(t) = A\cos(\omega t)$$

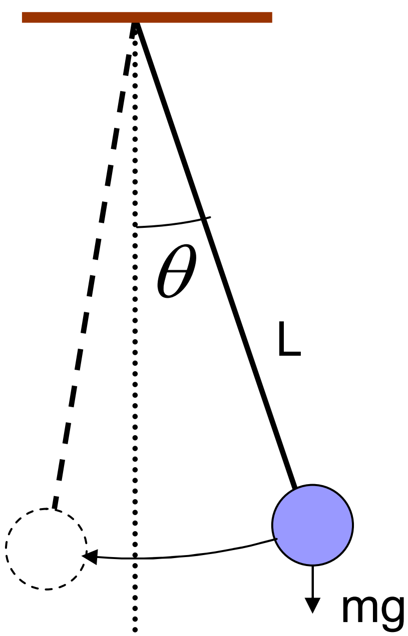
$$v(t) = -A\omega\sin(\omega t)$$

$$a(t) = -A\omega^2\cos(\omega t)$$

- What is the angular frequency in this case?
  - Use Newton's 2nd law, together with Hooke's law, and the above description of the acceleration to find:

$$\omega = \sqrt{\frac{k}{m}}$$

The simple pendulum



- Consider an object of mass m attached by a massless string of length L to a frictionless hinge. The torque exerted by gravity is

$$\tau = -mgL\sin\theta$$

- Newton's 2nd law for rotation: $\tau = I\alpha$
- $I=mL^2$, thus: $\alpha = -(g/L)\sin\theta$
- For *small angles*, $\sin\theta \approx \theta$,thus $\alpha = -(g/L)\theta$
- Recall for a spring: $a = -(k/m)x$
- Thus, by analogy we can see that for small angles the angle θ will undergo simple harmonic motion

$$\theta = \theta_0 \cos(\omega_p t)$$

with an angular frequency given by

$$\omega_p = \sqrt{g/L}$$

Simple Harmonic Motion

- A mass on a spring is one (and the most famous) example of *Simple Harmonic Motion*
- SHM is
- Any motion that can be described by a sinusoidal function: $x = x_m \cos(\omega t + \phi)$
- Any motion for which the acceleration is directly proportional to displacement, but in the opposite direction:

$$\frac{d^2x}{dt^2} = -\omega^2 x$$

- The behavior of one dimension of circular motion

Energy and Simple Harmonic Motion

- an ideal spring exerts a *conservative force* on the object attached to it
  - consider a object attached to the spring, and assume there are no other external forces acting on the object. Let the position and velocity of the object be given by:

$$x(t) = A\cos(\omega t) \qquad v(t) = -A\omega\sin(\omega t)$$

  - then, from the work-energy theorem, we know that the work done by the spring force is equal to the change in kinetic energy of the object:

$$W = \Delta KE = \frac{1}{2}mv_f^{\,2} - \frac{1}{2}mv_i^{\,2} = \frac{1}{2}mA^2\omega^2\left(\sin^2(\omega t_f) - \sin^2(\omega t_i)\right)$$

  - Consider the work done going through 1 cycle: $t_f = t_i + T = t_i + 1/f = t_i + 2\pi/\omega$

$$W = \frac{1}{2}mA^2\omega^2\left(\sin^2(\omega t_i + 2\pi) - \sin^2(\omega t_i)\right) = 0$$

  - a cycle is a *closed path* … and recall that this is one of the equivalent definitions of a conservative force: *the net work done by a conservative force moving an object around a close path is zero.*

Energy and Simple Harmonic Motion

- we know that a conservative force has a potential energy associated with it
- the work that a conservative force does when acting on an object is equal to *minus* the change in the corresponding potential energy …. from this we can deduce that the potential energy of an object attached to a spring is:

$$PE_s = \frac{1}{2}kx^2$$

- the total mechanical energy of the object (excluding rotation and gravity for now) is therefore:

$$E = \frac{1}{2}kx^2 + \frac{1}{2}mv^2$$

  - in the spring's unstretched position, x=0, and all of the energy is in the kinetic energy of the object
  - at the spring's maximum extension or compression, v=0, and so all the energy is potential energy
  - the potential energy of the mass is equal to the elastic energy stored in the spring coils

Total mechanical energy

- For an object attached to a spring and in the earth's gravitational field, its total mechanical energy is

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 + \frac{1}{2}I\omega^2 + mgh$$

- If the net external forces and net external torque (excluding those exerted by the spring and gravity) on the object is zero, then its total mechanical energy is conserved.

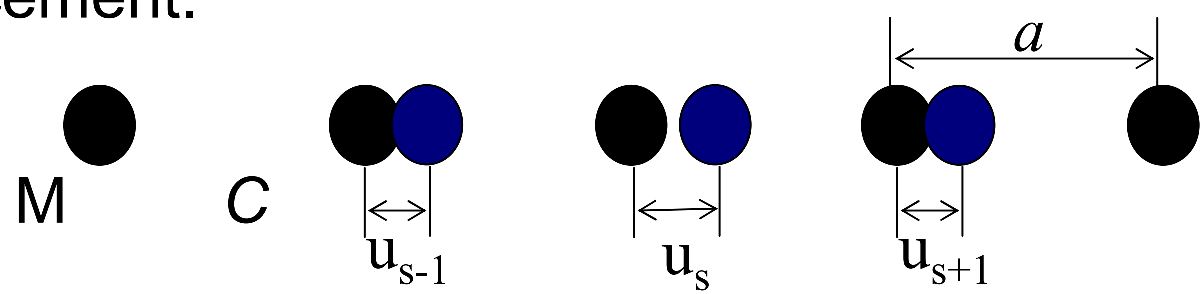
Quantum Harmonic Oscillators

A. Vibrations of the crystalline lattice
B. Motion of electrons in a Magnetic Field

Monoatomic Lattice

❑ Dispersion Relation Derivation

The assumption here is that the elastic response of the solid is a linear function of the forces, which means that the elastic energy is a quadratic function of the displacement.



According to Hooke's law, the total force on plane s is caused by the displacement of planes (s-1) and (s+1), i.e.

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

where *C* is a force constant between *n.n*. planes.

The equation of motion of plane s is then

$$M\frac{d^2u_s}{dt^2} = C\left(u_{s+1} + u_{s-1} - 2u_s\right)$$

For the case of a harmonic response in both space and time, i.e when

$$u_s(x,t) = ue^{isKa}e^{-i\omega t}$$

we arrive at the following dispersion relation

$$\boxed{\omega = \sqrt{\frac{4C}{M}}\left|\sin\left(\frac{Ka}{2}\right)\right|}$$

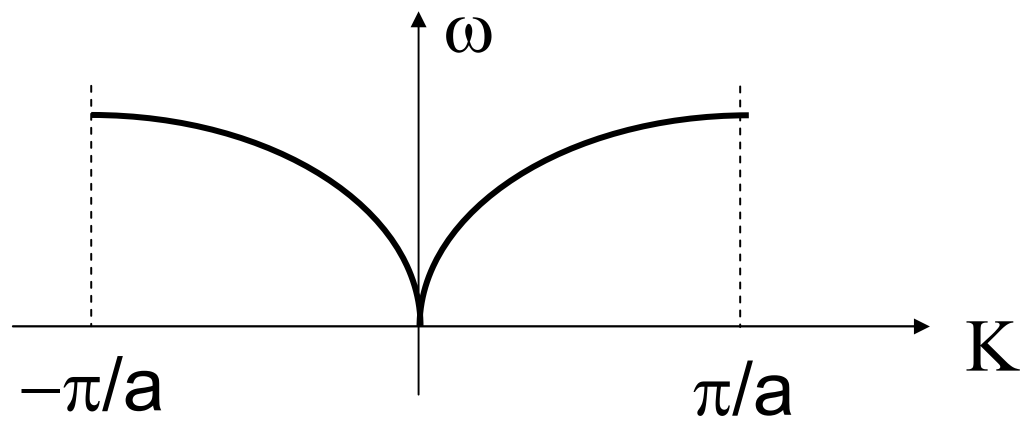
The significant wavevectors are found from:

$$\frac{u_{s+1}}{u_s} = \frac{ue^{i(s+1)Ka}}{ue^{isKa}} = e^{iKa}$$

$$= e^{i2\pi n}e^{ia(K-2\pi n/a)} = e^{iaK'}$$

$$\Rightarrow \quad -\pi/a \le K \le \pi/a$$

A graphical representation of the dispersion relation is shown in the figure below:



- At the zone boundaries, the group velocity of the waves is:

$$v_s = \frac{d\omega}{dK} \rightarrow v_s(K = \tfrac{\pi}{2}) = \sqrt{\frac{Ca^2}{M}} \cos(\pi/2) = 0$$

- In the long wavelength limit *K*a<<1, we have that the velocity of the sound is independent of frequency, i.e.

$$\omega \approx a\sqrt{\tfrac{C}{M}}K = v_s K$$

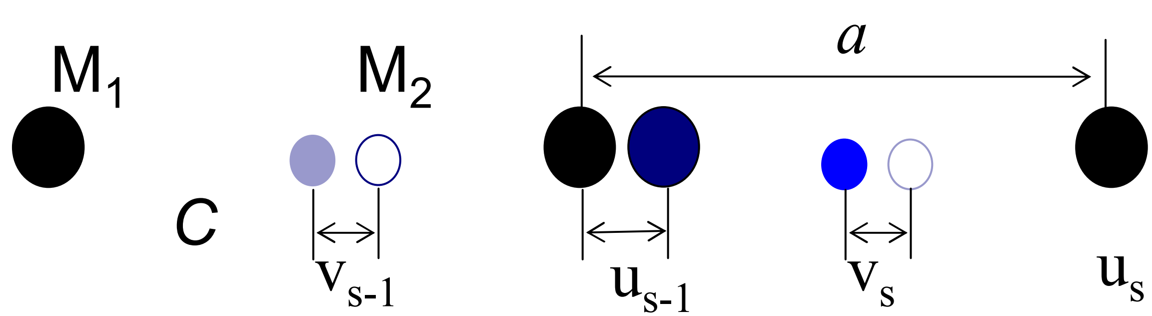
Two Atoms per Primitive Basis

❑ Dispersion relation derivation

For the case when there are p-atoms in the primitive cell, there are 3p branches out of which:

- 3 = acoustical branches: 1 LA and 2 TA branches
- 3(p-1) = optical branches: (p-1) LO and 2(p-1) TO

The problem we consider now is of a diatomic lattice with two atoms per basis with masses M_1 and M_2



The equations of motion are:

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

Again, for the case of harmonic response we arrive at a following set of equations written in a matrix form:

$$\begin{bmatrix} 2C - M_1\omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2\omega^2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = 0$$

The homogeneous set of equations has non-trivial solutions when the determinant of the matrix is zero, that leads to the following dispersion relation

$$M_1 M_2 \omega^4 - 2(M_1 + M_2)C\omega^2 + 2C^2[1 - \cos(Ka)] = 0$$

The exact solutions to this equation can be found, but it is simpler to consider the two separate cases when Ka<<1 (long wavelength limit) and the case when Ka=$\pm\pi$ (at the boundary)

(a) Case Ka<<1 (long wavelength limit)

In this first case the two solutions are of the form:

$$\omega_1^2 \approx 2C\left(1/M_1 + 1/M_2\right) = const.$$

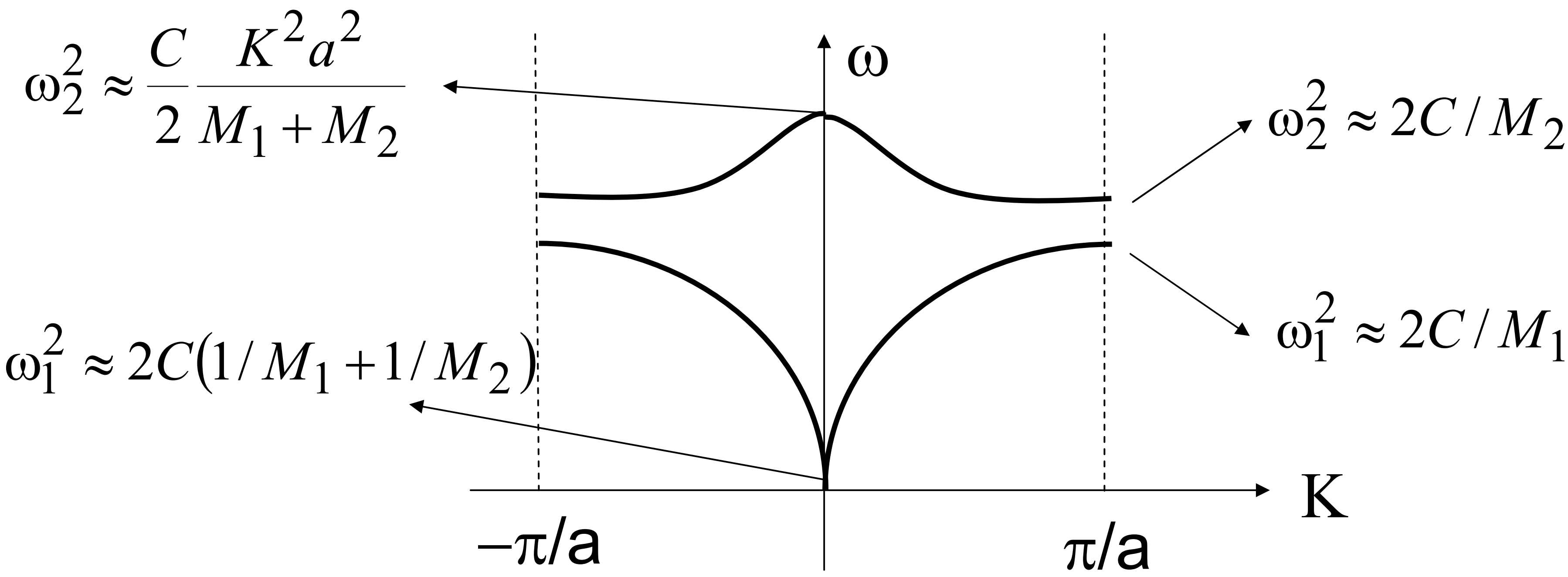
$$\omega_2^2 \approx \frac{C}{2}\frac{K^2a^2}{M_1 + M_2}$$

(b) Case Ka= $\pm\pi$ (at the boundary)

In this second case the two solutions are of the form:

$$\omega_1^2 \approx 2C/M_2$$

$$\omega_2^2 \approx 2C/M_1$$



◎ For Ka<<0 (long wavelength limit) and $\omega=\omega_2$, we have:

- One lattice wave to be moving against the other lattice, i.e.

$$u/v = -M_2/M_1$$

- One can excite this mode with light waves – optical branch.

◎ For Ka= $\pm\pi$, we get that the two lattices are completely decoupled from each other.

Quantization of the Elastic Waves

The **energy of lattice vibration** a is quantized, and the quantum of energy is called a **phonon**, in analogy to photons for quantization of the electromagnetic waves.

The energy of an elastic mode of vibration describing a state of n-phonons is given by:

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega$$

To calculate the energy of the mode, one starts from the harmonic approximation for the displacement

$$u_s(x,t) = U_0 e^{isKa} e^{-i\omega t}$$

The energy in a mode then equals ½ kinetic and ½ potential energy. The kinetic energy is given by:

$$K.E. = \frac{1}{2}\rho\left(\frac{du}{dt}\right)^2 = \frac{1}{2}\rho U_0^2\omega^2\cos^2(Kx)\sin^2(\omega t)$$

$$\rightarrow \left(\text{after spatial and temporal integration}\right)$$

$$\rightarrow \frac{1}{8}\rho V\omega^2 U_0^2$$

When equating the two expressions, we get:

$$\frac{1}{2}\left(n+\frac{1}{2}\right)\hbar\omega = \frac{1}{8}\rho V\omega^2 U_0^2$$

$$\rightarrow U_0 = 2\sqrt{\frac{(n+1/2)\hbar}{\rho V\omega}}$$

To summarize, the amplitude of the oscillation U_0 is proportional to the square root of the number of phonons in a given mode.

The Phonon Momentum

In here we give the discussion that phonons do not carry any momentum, but for all practical purposes, one can consider that phonons are particles that have:

- large momentum, and
- small energy, on the order of 30 to 80 meV .

The equation that governs the conservation of momentum is of the form:

$$\mathbf{k}' \pm \mathbf{K} = \mathbf{k} + \mathbf{G}$$

where the ± sign is for the phonon creation/annihilation (absorption) process and **G** is the reciprocal lattice vector.